# Detection of Adulterants in Raw Materials Utilizing Hyperspectral Imaging with Target and Anomaly Detection Algorithms

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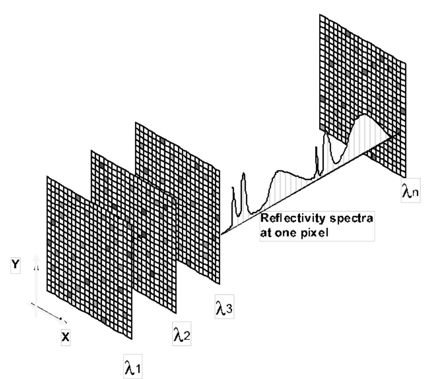
NIR hyperspectral reflectance imaging is an important exploratory and analytical tool for many industries including precision agriculture, food production, chemical processing and pharmaceutical manufacturing. The combination of spatial and spectral information creates unique capabilities for revealing complexities of both natural and man-made materials because the multi-pixel measurements provides a more sensitive and representative sampling of powder materials. In this paper, we focus on the application of hyperspectral imaging with target and anomaly detection algorithms for detection of adulterants in raw materials used in the food industry. NIR reflectance hyperspectral images were obtained using OPOTEK's tunable laser as the illumination source. The tunable laser replaces broadband light source and filters commonly used in alternative technologies and results in better signal-to-noise ratio, higher spectral resolution and fast data acquisition rates. The detection algorithms were designed to adapt to variable background matrices (a.k.a., clutter) while maintaining high sensitivity to anomalies and target signal attributable to known adulterants. The demonstrated fast detection and classification at ppm levels has significant positive implications for inspection of raw materials in the food industry and can easily be extended to other applications.

# Objective

- Detection of adulterants in raw materials using hyperspectral imaging
- Anomaly detection – finds unusual signal
- Target detection – finds unusual signal specific to a target spectrum
- Examples
  - explosive residue on a cellulosic swipe
  - melamine in wheat gluten at multiple concentrations

# What is Spectral Imaging? Why?




Spectral (chemical information)
AND
Images (spatial information)

- Function derives from spatial composition
  - Both "what" and "where" are important
- Non-destructive; fast

# HySPEC™

## Hyperspectral Imaging with Tunable Laser Illumination


OPOTEK

| Attribute | Effect | Advantage |
|---|---|---|
| Wide Tuning Range | | 410 – 2400nm |
| Narrow Spectral Linewidth | | High Spectral Resolution (1 – 2.5nm) |
| Short Pulse (5ns) | Short Integration Time | Camera Gating<br>Not affected by Ambient Light |
| High Intensity | Single frame data acquisition | Short scan time<br>Large FOV |
| Low Avg. Power | Sample not subjected to heat | No sample damage |
| Wavelength Measurement | Real-time calibrated wavelength | High spectral accuracy |
| Fiber Delivery | Easy and efficient light delivery | Flexible configurations |

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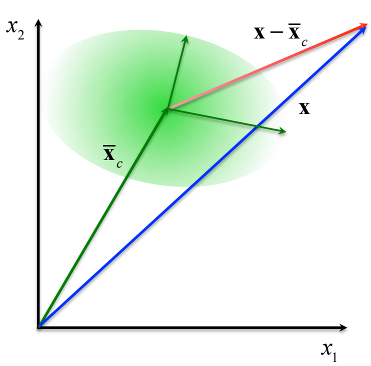
# Anomaly Detection I

- Detect unusual signals relative to normal (or null) signal.




- Hotelling's $T^2$ is a measure from the data center relative to the null covariance.
  - It can be thought of as a multivariate extension of a t-test.
  - Regularization can be used to estimate the inverse.

$$T^2 = \left(\mathbf{x} - \bar{\mathbf{x}}_c\right)^T \mathbf{W}_c^{-1} \left(\mathbf{x} - \bar{\mathbf{x}}_c\right)$$

$\mathbf{x}$ is a new measurement

$\bar{\mathbf{x}}_c$ is the null mean

$$\mathbf{W}_c = \tfrac{1}{M_c - 1}\left(\mathbf{X}_c - \mathbf{1}\bar{\mathbf{x}}_c^T\right)^T \left(\mathbf{X}_c - \mathbf{1}\bar{\mathbf{x}}_c^T\right)$$

is the null covariance

Hotelling, H. (1931). "The generalization of Student's Ratio." *Annals of Mathematical Statistics* **2** (3), 360-378.

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# Anomaly Detection II

- Principal Components Analysis (PCA)
    - often used for anomaly detection and multivariate statistical process control
  - uses $T^2$ on scores and limits on residuals.[1]
  - Other models include maximum autocorrelation factors and maximum difference factors.[2]
- Detects anomalies but requires additional interrogation to attempt to classify
  - determine why was the signal unusual.

[1]Wise, B.M. and Gallagher, N.B., "The Process Chemometrics Approach to Chemical Process Monitoring and Fault Detection," *J. Proc. Cont.* **6**(6), 329-348 (1996).

[2]Blake, T.A., Kelly, J.F., Gallagher, N.B, Gassman, P.L., Johnson, T.J., "Passive Detection of Solid Explosives in Mid-IR Hyperspectral Images," *Anal. Bioanal. Chem.*, **395**(2), 337-348 (2009).

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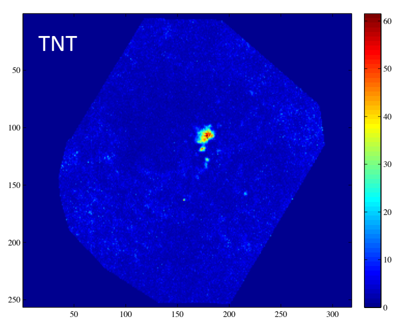
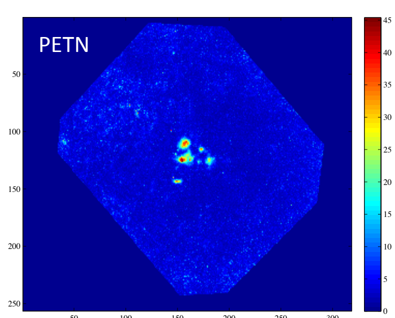
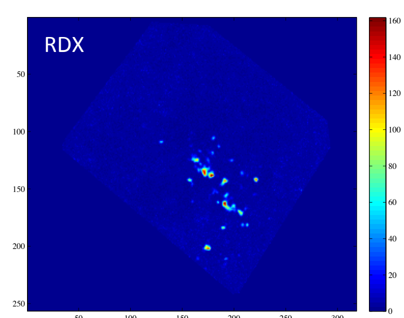
# Anomaly Detection for Explosive Residue on Swipes



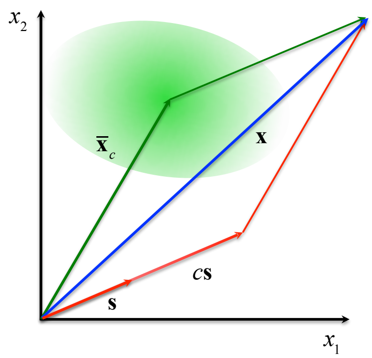

Klunder, G., Nguyen, L. K., Margalith, E., "Near infrared spectral imaging of explosives using a tuneable optical parametric oscillator laser source," NIR News, 22(3), 19-21 (2011).



# Target Detection I

- Detect unusual signals relative to null signal in a specified target direction.




- Generalized least squares (GLS) is often used for target detection. A.k.a.,
  - Aitken Estimator,
  - Matched Filter, and
  - Adaptive Matched Filter.

$$\hat{c} = \left(\mathbf{x} - \bar{\mathbf{x}}\right)^T \mathbf{W}_c^{-1}\mathbf{s}\left(\mathbf{s}^T\mathbf{W}_c^{-1}\mathbf{s}\right)^{-1}$$

$\mathbf{s}$ is the target to the signal

$\hat{c}$ is the contribution of the target to the signal

Aitken, A. (1935) "On Least Squares and Linear Combinations of Observations", *Proceedings of the Royal Society of Edinburgh*. **55**, 42-48.

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# Target Detection II

- The model should be based on how the signal manifests e.g.,

Additive model

$$\hat{c} = \left(\mathbf{x} - \bar{\mathbf{x}}\right)^T \mathbf{W}_c^{-1}\mathbf{s}\left(\mathbf{s}^T\mathbf{W}_c^{-1}\mathbf{s}\right)^{-1}$$

Linear mixture model

$$\begin{bmatrix} \hat{c} & \hat{c}_c \end{bmatrix} = \mathbf{x}^T\mathbf{W}_c^{-1}\mathbf{z}\left(\mathbf{z}^T\mathbf{W}_c^{-1}\mathbf{z}\right)$$

$$\mathbf{z} = \begin{bmatrix} \mathbf{s} & \bar{\mathbf{x}}_c \end{bmatrix}$$

- Statistics used vary, but t-stat and F-stat are useful.
  - t- and F-statistics are calculated relative to the null

$$t = \frac{\hat{c} - \bar{c}_c}{\sigma_c}$$

$$Q = \left(\mathbf{x} - \hat{c}\mathbf{s}\right)^T \mathbf{W}_c^{-1}\left(\mathbf{x} - \hat{c}\mathbf{s}\right)$$

$$F = Q / Q_{CL}$$

$t$ is the t-statistic

$\bar{c}_c$ is the mean of contributions off-target

$\sigma_c$ is the std of contributions off-target

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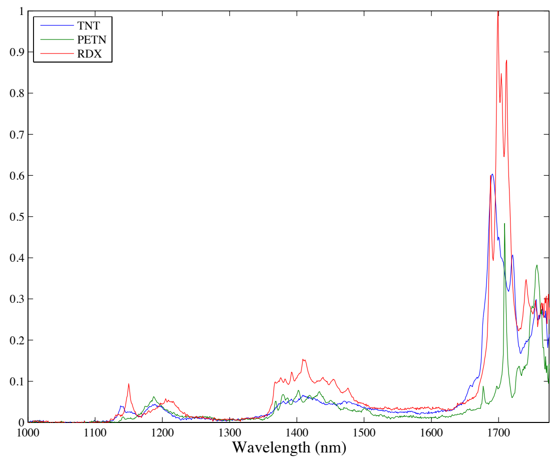
# Explosives Targets

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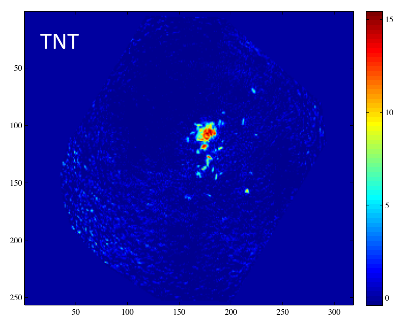
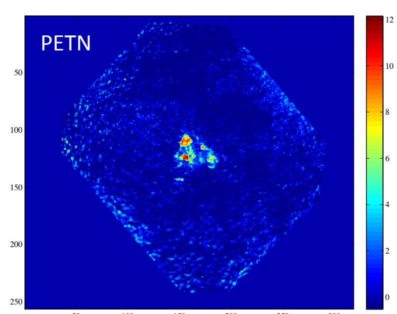
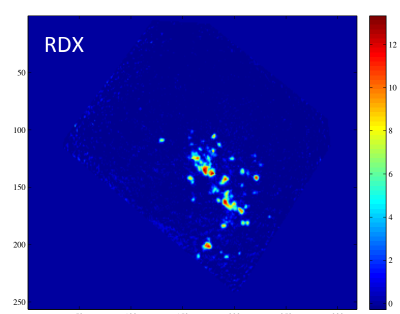
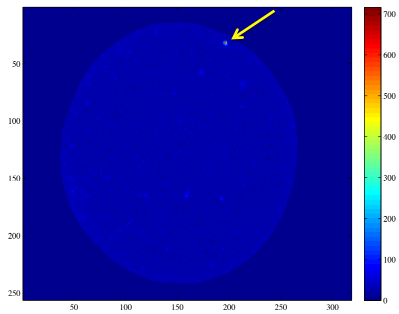



# Target Detection for Explosive Residue on Swipes



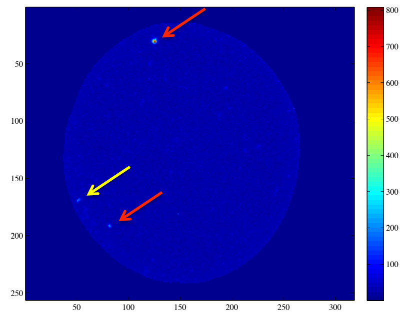



# Anomaly Detection for Melamine in Wheat Gluten



anomaly unrelated to melamine detected

M_in_G1_0000_01_20101028
0 ppm melamine



anomalies due to melamine and unrelated to melamine detected

M_in_G1_0200_02_20101027
200 ppm melamine

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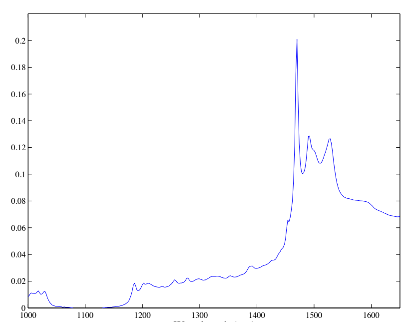
# Melamine Target

- Find melamine in wheat gluten
  - Sigma Aldrich Melamine 99%
  - M2659
  - CAS 108-78-1
- 0, 11, 23, 56, 100, 200, 500, 1000 ppm
  – five replicates each




median of two melamine samples
-log(R) and baselined

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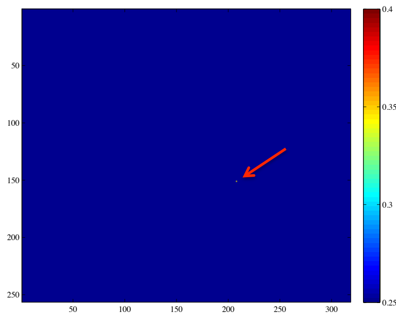
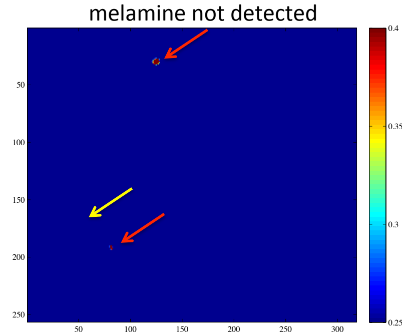
# Target Detection for Melamine in Wheat Gluten

target detected in a single pixel



M_in_G1_0056_01_20101027
56 ppm melamine

target melamine detected
anomaly unrelated to melamine not detected



M_in_G1_0200_02_20101027Anomaly
200 ppm melamine

# “ground truth table” for detection of melamine in wheat gluten

| Image (ppm) | Number of Detected Pixels known | Number of Detected Pixels target |
|---|---|---|
| M_in_G1_0000_01 | 0 | 0 |
| M_in_G1_0000_02 | 0 | 0 |
| M_in_G1_0000_03 | 0 | 0 |
| M_in_G1_0000_04 | 0 | 0 |
| M_in_G1_0000_05 | 0 | 0 |
| M_in_G1_0011_01 | | 0 |
| M_in_G1_0011_02 | | 0 |
| M_in_G1_0011_03 | | 0 |
| M_in_G1_0011_04 | | 0 |
| M_in_G1_0011_05 | | 0 |
| M_in_G1_0023_01 | | 0 |
| M_in_G1_0023_02 | | 0 |
| M_in_G1_0023_03 | | 0 |
| M_in_G1_0023_04 | | 0 |
| M_in_G1_0023_05 | | 0 |

| Image (ppm) | Number of Detected Pixels known | Number of Detected Pixels target |
|---|---|---|
| M_in_G1_0056_01 | ~1 | 1 |
| M_in_G1_0056_02 | 0 | 0 |
| M_in_G1_0056_03 | 0 | 0 |
| M_in_G1_0056_04 | 0 | 0 |
| M_in_G1_0056_05 | 0 | 0 |
| M_in_G1_0100_01 | 0 | 0 |
| M_in_G1_0100_02 | 0 | 0 |
| M_in_G1_0100_03 | 0 | 0 |
| M_in_G1_0100_04 | ~12 | 7 |
| M_in_G1_0100_05 | 0 | 0 |
| M_in_G1_0200_01 | ~10 | 6 |
| M_in_G1_0200_02 | ~70 | 49 |
| M_in_G1_0200_03 | 0 | 0 |
| M_in_G1_0200_04 | 0 | 0 |
| M_in_G1_0200_05 | 0 | 0 |
| M_in_G1_0500_01 | ~13 | 18 |
| M_in_G1_0500_02 | ~40 | 17 |
| M_in_G1_0500_03 | 0 | 0 |
| M_in_G1_0500_04 | ~45 | 33 |
| M_in_G1_0500_05 | ~ 8 | 6 |
| M_in_G1_1000_01 | | 70 |
| M_in_G1_1000_02 | | 103 |
| M_in_G1_1000_03 | | 187 |
| M_in_G1_1000_04 | | 62 |
| M_in_G1_1000_05 | | 121 |

# Conclusions

- Anomaly detection finds unusual pixels in an image
  - simple, but the reason for the anomaly requires interrogation
- Target detection provides classification as part of the algorithm
  - more easily used in automated environments
  - examination of residuals can also be used for anomaly detection – and subjected to additional target analysis
- Hyperspectral imaging is useful for detection of adulterants for heterogeneous samples
  - however, the adulterant needs to be at, or near, the surface of the sample

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